



Sources and propagation of uncertainty in N₂O model predictions

Domingo Felez, Carlos; Valverde Pérez, Borja; Plósz, Benedek G.; Sin, Gürkan; Smets, Barth F.

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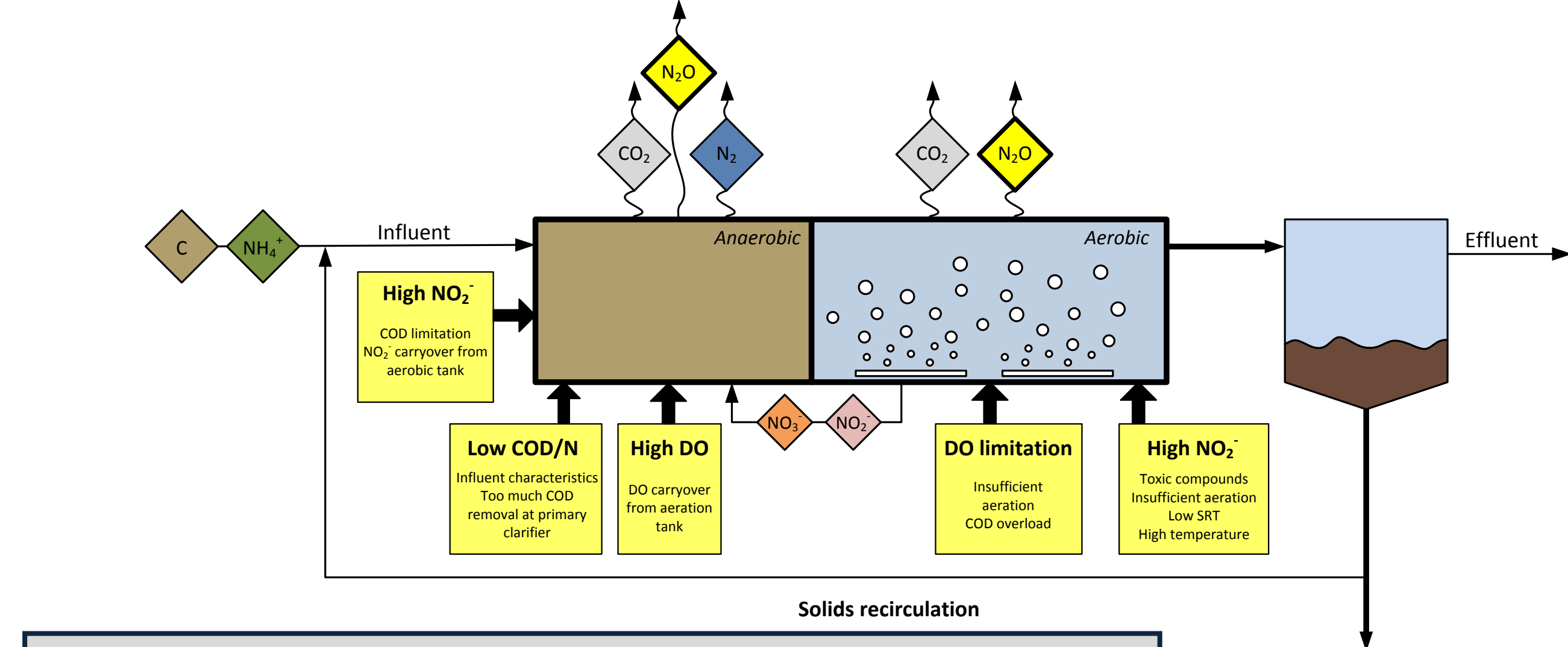
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1. Introduction and research questions

Nitrous oxide emissions during nitrogen removal in wastewater treatment operations can compromise the environmental impact of the process.

The carbon footprint of a WWTP is highly sensitive to N₂O emissions.

Model predictions carry uncertainty from the calibration process.

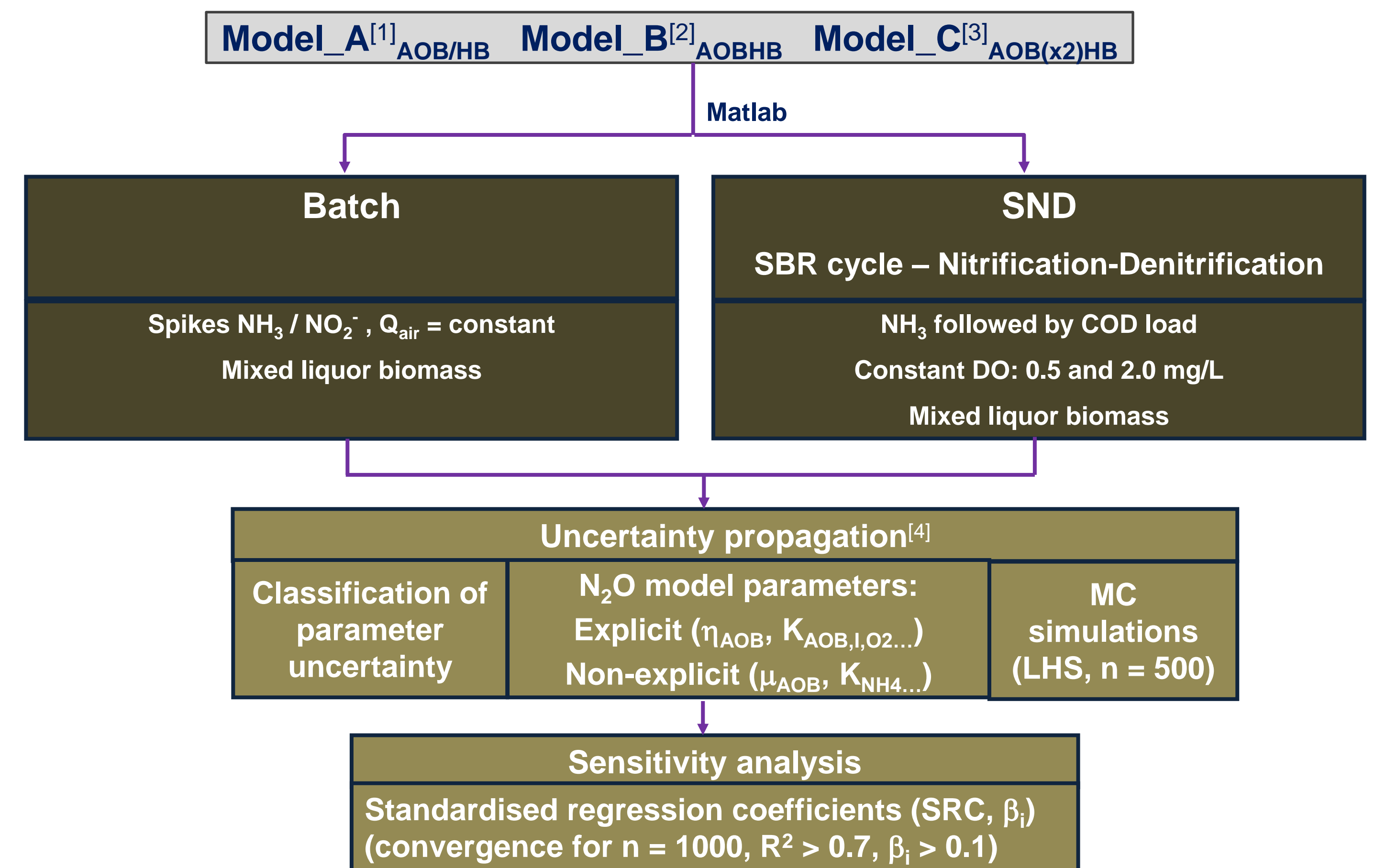


Q1. How precise are N₂O model predictions?

Q2. Are calibration results satisfactory for mitigation strategies?

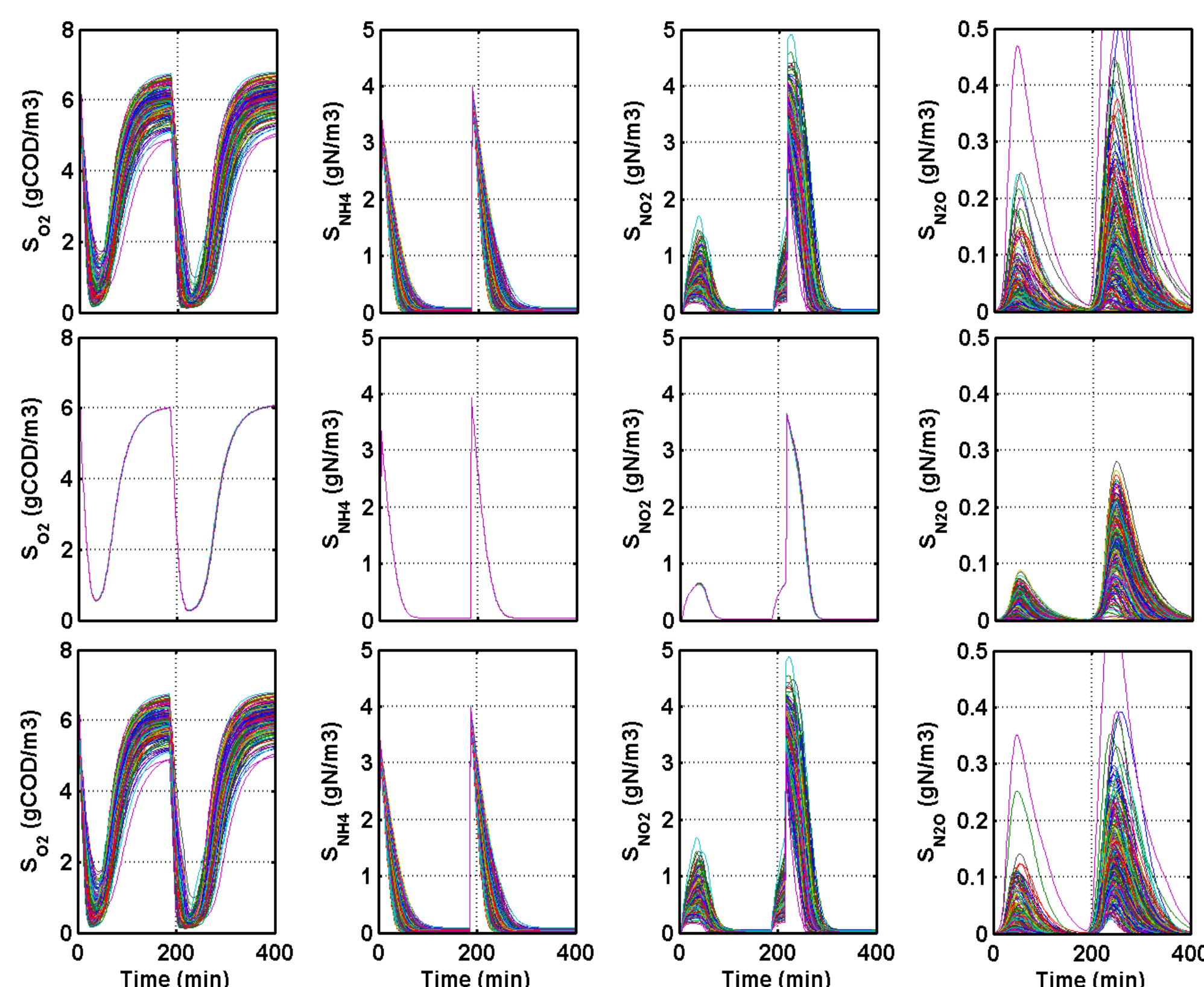
Q3. How can we reduce the uncertainty of model predictions?

2. Computational work performed



3. Uncertainty in model predictions

Model predictions if uncertainty is considered for Model_A, Batch:



All parameters

Parameters specific to N₂O

Parameters specific to not N₂O

Model predictions for N₂O carry higher uncertainty associated to previous processes.

Higher coefficient of variation for N₂O compared to DO, NH₄⁺, NO₂⁻ along the experiment.

What parameters carry most of the uncertainty?

Batch

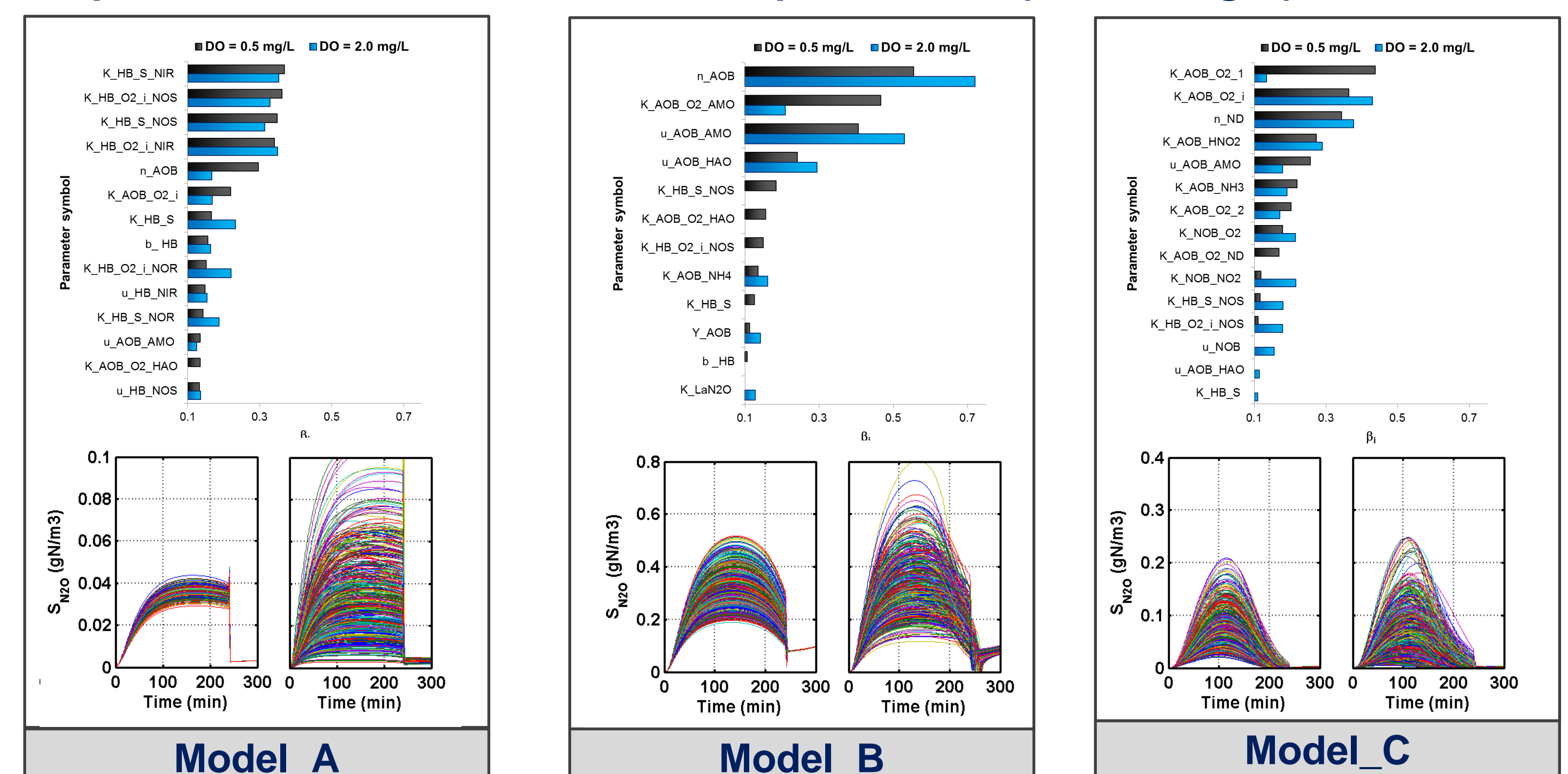
4. Identifying sources of uncertainty

Model evaluation with reported parameter values, scenario SND

	DO = 0.5 mg/L			DO = 2.0 mg/L		
	Model_A	Model_B	Model_C	Model_A	Model_B	Model_C
ΔNH ₄ (mgN/L)	29	26	25	35	38	39
N ₂ O _{emitted/removed}	2.1%	2.3%	4.8%	0.4%	3.6%	0.5%
NN	-	95%	1%	-	99%	4%
N ₂ O _{prod}	ND	58%	91%	ND	67%	82%
HD	42%	5%	8%	33%	1%	14%

Ranking of the most sensitive parameters for each model/scenario

Propagation of uncertainty for: reported parameters (bottom left), and reported + sensitive non-calibrated parameters (bottom right)



For the 3 models considered N₂O emissions were sensitive to non-explicit N₂O parameters from AOB and HB.

Calibration efforts for sensitive parameters can reduce the prediction uncertainty (Calibrated parameters: Model_C = 11, Model_A = 5).

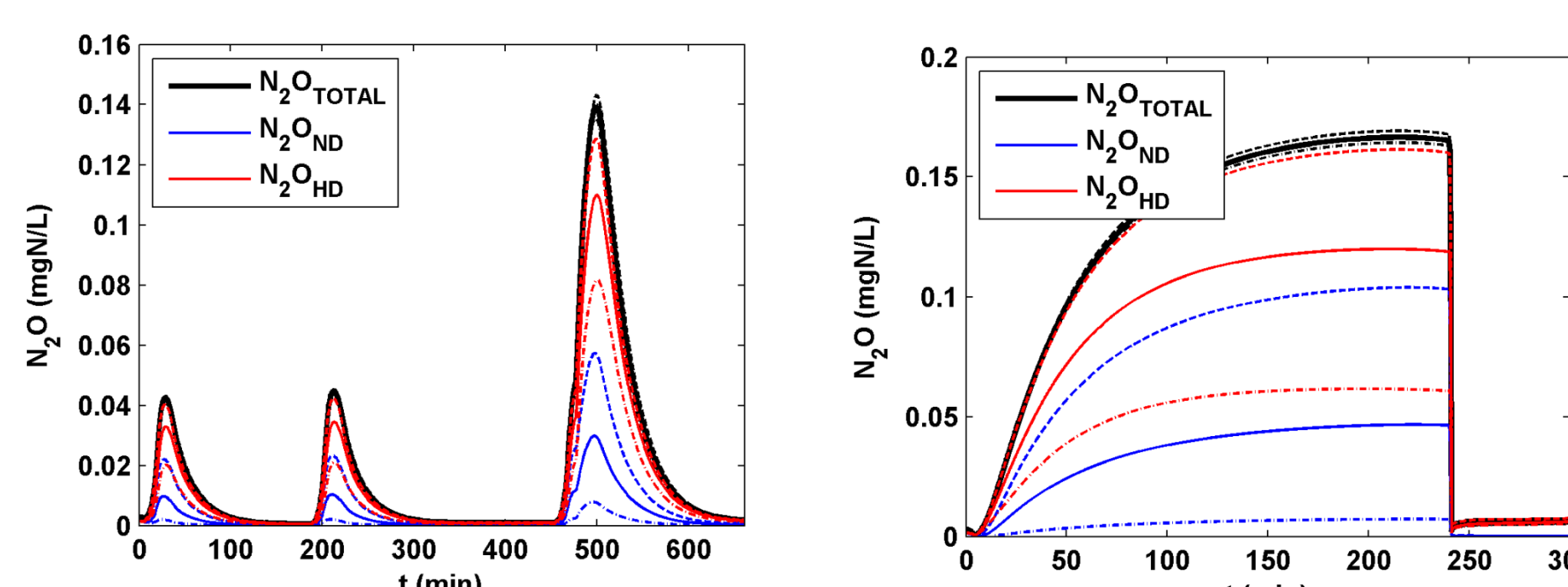
SND

5. Total vs Individual pathway contribution

Strategies to mitigate N₂O emissions are pathway-dependent.

Are individual N₂O production pathways sensitive to the same parameters as total N₂O?

Uncertainty in non-sensitive parameters to total N₂O revealed poor identifiability of individual pathway contributions.



Batch

SND

Effect of varying non-sensitive parameters to N₂O predictions (black) and to individual pathway contributions (red, blue) (95% CI dashed lines. K_{HB,NO}, K_{AOB,NO}: 0.02 mgN/L ± 90%)

6. Conclusions – Outlook

- Uncertainty of N₂O emissions is related to both explicit and non-explicit N₂O model parameters.
- N₂O model calibrations should systematically address sensitivity and identifiability problems due to uncertainty propagation from previous processes.
- Adequate experimental design for model calibration can significantly reduce uncertainty of parameter estimates and therefore prediction uncertainty.
- Precise N₂O predictions might underestimate uncertainty of individual pathway contributions.